Resource Department

GEOCHEMISTRY

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The Earth Sciences Division's Geochemistry Department combines expertise in chemical and isotopic analysis, molecular geochemistry and nanogeoscience, mineralogy, and multiscale data-gathering methodology to enable geochemical characterization of earth systems from the macroscopic to the molecular. The department comprises four groups with complementary interests and capabilities.

MOLECULAR GEOCHEMISTRY AND NANOGEOSCIENCE

Studies in this group address issues of contaminant sequestration and migration in the environment, mineral-fluid reactions, and various aspects of aqueous solution chemistry. Fundamental studies on the nature of the aqueous solution/mineral interface and on the structure of (near-aqueous) solvated ions and colloids down to the nanometer regime are also being performed. The aim of the latter studies is to provide improved modeling capability for contaminant migration, weathering, sediment transfer, ion exchange, and nutrient cycles. Current work includes: molecular-dynamics modeling of the interlayer-solvated cations in clays and the aggregation dynamics of nanoparticle iron oxides; studies of the solvation environment of contaminant and nutrient molecules in aqueous solution; determination of the molecular identity of initial iron oxide precipitates on quartz surfaces; and characterization of the surface chemistry and structure of environmentally important minerals via simulation, x-ray scattering, and x-ray spectroscopy methods. Many of these efforts involve newly developed capabilities utilizing synchrotron x-ray sources. Important new work on the aqueous behavior of humic and fulvic acids, hydroxyl speciation near cations in water, and the nature of organic contaminants on mineral surfaces has been carried out recently at Berkeley Lab's Advanced Light Source. The group also does extensive collaboratory research utilizing the NCEM at Berkeley Lab, and takes advantage of the NSERC facility at Berkeley Lab for large-scale molecular dynamics simulations.

ISOTOPE GEOCHEMISTRY

The Isotope Geochemistry group operates the Center for Isotope Geochemistry, which was established in 1988 and includes six important analytical facilities: stable isotope and noble gas isotope laboratories; a soil carbon laboratory; an analytical chemistry laboratory; the Inductively Coupled Plasma Multi-Collector Magnetic Sector mass spectrometry laboratory, and a thermal-ionization mass spectrometry laboratory located on the UC Berkeley campus. We also have an affiliation with the cosmogenic isotope laboratory in UC Berkeley's Space Sciences Laboratory. These facilities provide state-of-the-art characterization of all types of earth materials for research throughout the department and elsewhere in the division. Further, they support the Center's goals of finding new ways to utilize isotopic ratio methods to study earth processes, and applying isotopic and chemical analysis procedures to specific environmental and energy problems of national interest.

Current research programs include: (1) the development of models that use isotopic composition data from element pairs in fluids to constrain fluid flow rates, water-mineral reaction rates, and the geometry and spacing of fractures in rock matrices; (2) the development and application of noble gas isotopes as natural tracers for fluid source and movement in hydrocarbon and geothermal systems; (3) development of techniques for dating Quaternary geological events using uranium-thorium-helium systematics; (4) the geochemical monitoring and analysis of large-scale experiments simulating the effects of nuclear waste heat generation within the proposed repository in Yucca Mountain, Nevada; (5) the application of helium and neodymium isotopes to determine magma-chamber recharge rates in areas having possible volcanic hazards or the potential for geothermal energy extraction; (6) the development of carbon, nitrogen, and oxygen isotope techniques for quantifying *in situ* bioremediation and environmental restoration; (7) the use of carbon isotopes to quantify rates of organic carbon cycling and storage efficiency in soils, the impact of climate change on carbon cycling, and linkages between carbon, water, and nitrogen cycles, (8) application of natural isotopic tracers to follow the movement of water and contaminates through the vadose zone and in groundwater, and (9) applications of hydrogen and oxygen isotopes to issues concerning the water cycle. A new program is under way to study iron isotope variations as a tracer in the oceanic and terrestrial iron cycles.

ATMOSPHERE AND OCEAN SCIENCES

The focus of this group is on the characterization of conditions and chemical components in the oceans and atmosphere, and on the development of process models using these inputs (combined with other hydrospheric data) to explain and predict climatic change.

The California Water Resources Research and Applications Center maintains a suite of research and operational tools for weather forecasts, climate prediction, and basic research. Ongoing collaborations include: streamflow simulations with the National Oceanic & Atmospheric Administration's California Nevada River Forecast Center; runoff contaminant monitoring and management with the U.S. Bureau of Reclamation; development of landslide-hazard prediction models with faculty at UC Berkeley; development of snow-cover and snow-water equivalent maps for California with UC Santa Barbara; and development of a shared information distribution system with the U.S. Department of Energy's Accelerated Climate Prediction Initiative (DOE/ACPI) collaborators. Outreach activities for this year have included a scientific exchange program with AmazonTech.

The central motivation for ocean science research in this group is to better understand the biological and physical processes governing carbon in the ocean, how these processes affect the balance of CO_2 between atmosphere and ocean, and the efficacy of using the oceans to sequester carbon. The issues are technologically challenging because of the rapidity of ocean biological processes—the entire carbon biomass in the ocean is replaced every one or two weeks.

The Berkeley Lab team collaborates with other scientists to deploy Carbon Explorers—robotic floats with telemetry capability and special sensors that can measure the distribution and fate of ocean carbon, as well as temperature, salinity, and pressure. In the laboratory, work is directed at expanding the sensor suite carried by Carbon Explorers. The latest innovation is an imaging optical sensor designed to simultaneously quantify the sedimentation of both inorganic and organic particulate carbon. The first Explorers documented the response of marine biota to iron deposited in the Pacific Ocean by a massive dust storm that had originated in Asia. In the Southern Ocean, Carbon Explorers have quantified biomass enhancement in response to deliberate iron addition to the ocean. A large-volume *in situ* filtration system is also used to collect size-fractionated particulate samples from surface to kilometer depths in the oceans.

GEOCHEMICAL TRANSPORT

A major effort of this group is the simulation and study of coupled mineral-water-gas reactive transport in unsaturated porous media. The work covers a wide range of processes under differing geologic environments, including infiltration/evaporation processes in the soil zone, reactive transport processes in fractured rock under boiling conditions, injection of CO_2 in deep aquifers, and hydrothermal alteration in geothermal systems. Although reactive transport modeling and code development are the predominant activities, the group is also active in planning the analysis and drilling activities for underground thermal experiments, laboratory experiments, and field studies of geothermal systems and natural analogues for nuclear waste isolation.

Much of the work is focused on predicting thermally driven processes accompanying the proposed emplacement of high-level nuclear waste at Yucca Mountain, Nevada, and on understanding the evolution of the natural hydrogeochemical system. The group has expanded its efforts to studies of geothermal systems, CO_2 sequestration, and modeling of stable isotope variations in the vadose zone. Collaboration among others in the division brings together essential pieces of the problem, including hydrological processes in the unsaturated zone, thermodynamics and kinetics of geochemical processes, and isotopic effects.

Current projects include:

- Simulation and analysis of an ongoing large-scale underground thermal test, and planning of future drilling and sampling efforts
- Prediction of coupled thermal-hydrological-chemical processes around potential waste emplacement tunnels to evaluate changes in water and gas chemistry, mineralogy, and flow
- Analysis of geochemical and isotopic data from Yucca Mountain, including ^{36}Cl as a bomb-pulse tracer, to constrain models of flow and transport in the unsaturated zone
- Development of models for reactive transport in unsaturated systems and co-developers of the reactive transport code TOUGHREACT
- Evaluation and development of improved thermodynamic and kinetic databases for water-rock interaction modeling, including new relations for CO_2 solubility to model CO_2 sequestration
- Research on natural analogue sites, including (a) analysis and modeling of continuously cored intervals from the Yellowstone geothermal system to assess effects of mineral alteration on fracture and matrix permeability; (b) study of flow, transport, and secondary mineralization at Peña Blanca, Mexico; and (c) study of anthropogenic analogues, such as those at the Idaho National Engineering and Environmental Laboratory
- Modeling of CO_2 sequestration in saline aquifers, including the impact of acid gas components, H_2S and SO_2, and interactions with shale confining beds
- Modeling hydrothermal alteration in geothermal systems.
- Simulation of the effects of scaling and acidization on permeability in geothermal injection wells at the Tiwi geothermal field, Philippines
- Study of chemical interaction between formation waters, injected waste fluids, and host rock during deep well injection
- Development of a Pitzer-type geochemical reactive transport model and simulation of high-ionic-strength groundwater contamination

FUNDING

Funding for the Geochemistry Department comes from a variety of sources within the U.S. Department of Energy, including: the Director, Office of Science, Office of Basic Energy Sciences, Divisions of Materials Sciences, Engineering and Geosciences; Office of Environmental Management, Office of Science and Technology; Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies, Office of Geothermal Technologies; Office of Biological and Environmental Research; and the Office of Civilian Radioactive Waste Management. Additional funding is provided by the U.S. Environmental Protection Agency; U.S. Navy; National Aeronautics and Space Administration, Office of Space Science and NASA Earth Enterprise; National Science Foundation, Office of Polar Programs; the University of California Campus-Laboratory Collaboration Hydrology Project; National Oceanographic Partnership Program (administered by the Office of Naval Research); National Oceanic and Atmospheric Administration, Office of Global Programs of the U.S. Department of Commerce, and the Laboratory-Directed Research and Development (LDRD) Program at Berkeley Lab.